Corrections of experimental data given in computational formats.

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Usage of experimental data for applications often requires to correct (modify) data given in original publication and compiled to EXFOR database according to modern scientific knowledge, experience of an evaluator, or to some additional assumptions. Some evaluators have their own systems allowing necessary data modifications. Real example of such specific correction system was demonstrated by K.Zolatarev (IPPE, Russia) under IRDF-2002 project. The IAEA project "EXFOR Data Correction System" is an attempt to generalize specific solutions and to build a universal system - tools allowing implementation of typical data modifications with final goal to collect real corrections provided by experienced evaluators to a common database, preserving their knowledge and sharing it with all IAEA users.

First version of the system is already implemented. One of major requirements to the system is very simple syntax encouraging people to use it. This paper describes syntax of modifications (corrections) of experimental data in computational formats C4 and TABLE/XREF with following propagation to data processing codes and presentations (including plots, tables, comparison with evaluated data, etc.) in NDS Web retrieval system: http://www-nds.iaea.org/exfor/. The system does syntax analysis of corrections and produces a report of all performed operations.

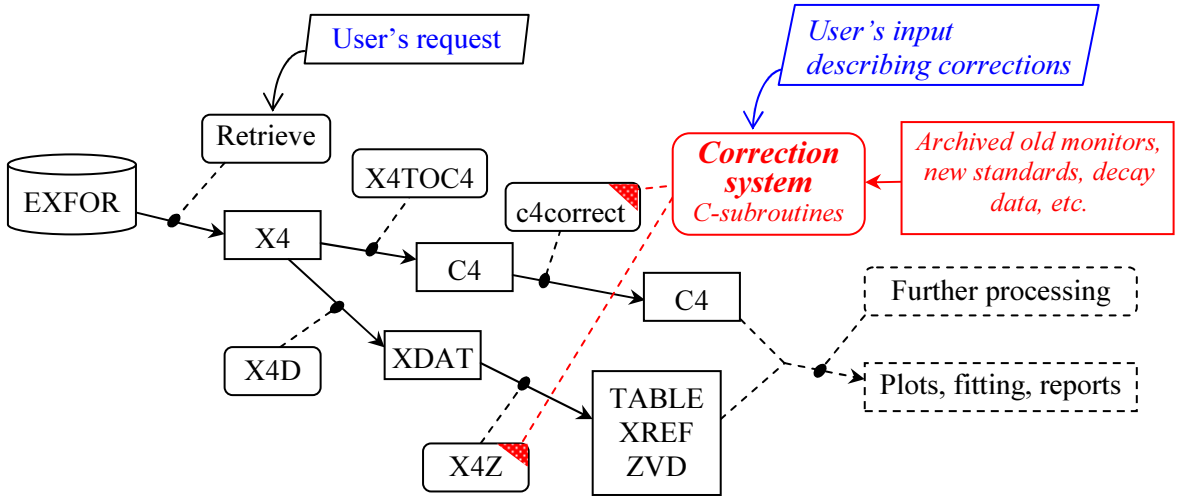


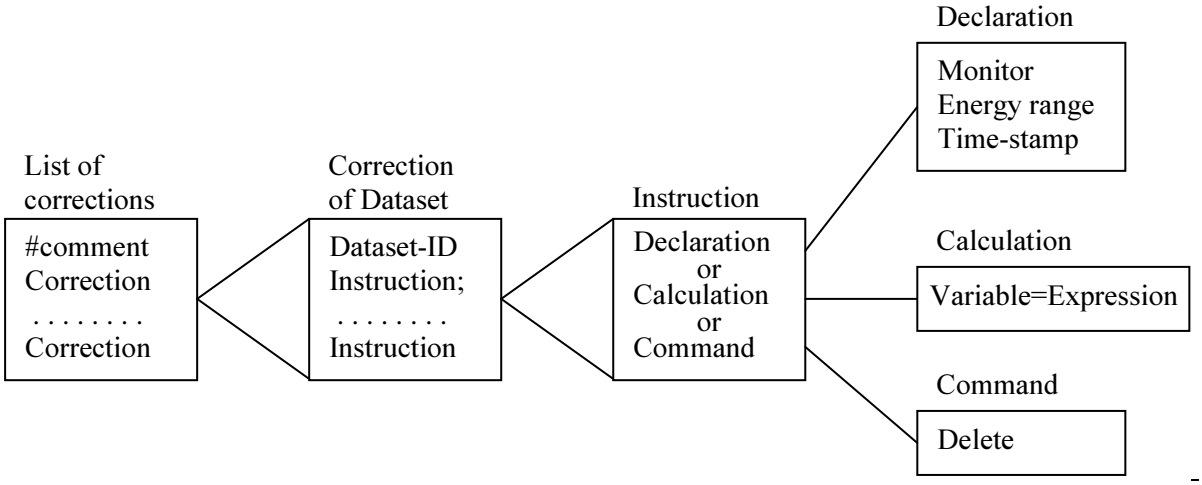
Fig.1 Structure of the system: data flows and programs

Corrections are described as sequence of instructions causing cascade of simple calculations of data in given data point of given dataset. There are three types of instructions: declarations, commands and data corrections. Instructions are implemented sequentially, so that result of an instruction can influence to the next calculation. Using logical names user describes corrections, for example: `E` - incident energy, `dE` - uncertainty of incident energy, `Y` - data (cross section, angular distribution, etc.), `dY` - data uncertainty, `m0, m1` – values of monitor cross sections for energy in given experimental point. Example of correction: `Y=Y/m0*m1` means renormalize data, i.e. for every experimental point: divide data value to old monitor value and multiply to new monitor value. Full description of modifications is given in the Table.1.

For the moment, the "correction-system" is able to perform:

- simple data re-calculation using given factor;
- re-calculate any numbers (including data, energies, angles and their uncertainties) by inter-data expressions using several math operations;
- any manipulations can be limited by an energy range;
- re-normalize data using monitors from archive and recent standards;
- re-normalize data using monitor data coded in EXFOR and recent standards;
- re-normalize data using isotopes abundances and half-lives;
- set up uncertainties if they are not given;
- delete part of a data set;
- convert ratios to absolute numbers;
- calculate ratios to archival monitors and to monitors coded in EXFOR;
- change incident energies;
- correcting wrong units, etc.

Corrections are given in a "List of corrections" – just sequential text describing corrections of one or many datasets. Corrections of every dataset must start from new line; they can be described in one line (separated by semicolon) or in many lines. The list of corrections can be stored (copy-paste) in a user's text file or database. The list has the following structure:



Variables.

There are two types of variables: parameters of experimental data point (energy, cross section, angle, uncertainties, MF, MT) and temporary variables (e.g. a0, a1, c0, c4, Fc). Values of variables can be used for calculations, and can be also changed (by =).

Numerical values.

These values can be used in expressions in the format of REAL numbers in Fortran. It is assumed that values without units are presented in "basic" units (e.g. 20. means 20eV). Expressions allow also usage of units (which must be presented in special working dictionary), then units will be replaced by factor, e.g. `2hr` will be replaced by `(2*3600)`.

Energy dependent monitor

Energy dependent monitor must be "declared" before first time used. Syntax: M1:Library$Reaction, e.g. m1:std05$u235nf. File identified by Library-Reaction with monitor cross section data should be present in internal Archive (including collection of old monitors and standards and latest standards). After that, monitor value for given energy can be used in expressions simply as m1. Monitor value will be approximated using monitor data around given energy.

Energy dependent monitor from EXFOR.

Monitor data can also be present as data in EXFOR file. Then in the correction system it can be declared as M0:[EN,MONIT], where EN and MONIT are headers in EXFOR DATA section. After that, monitor value for given energy can also be used in expressions simply as m0. For example, EXFOR-11420002 has MONITOR (92-U-235(N,F),,SIG) and monitor data are given in DATA section. Then renormalization of absolute data to the IAEA standard 2005 can be coded as:

```
11420002 m0:[EN,MONIT]; m1:std05$u235nf; y=y*m1/m0;
```

When incident energy should be averaged from two EXFOR columns it should be coded using "!" separating column-names, e.g.:

```
22816007  m0:[EN-MIN ! EN-MAX, MONIT]; m1:std05$au197ng;  y=y*m1/m0;
```

Monitor point.

Monitor value for given point (e.g. thermal cross section) can be used in an expression without declaration Library$Reaction[Energy], e.g. a1=iaea05$au197ng[0.0253].
It is also possible to use energy value from COMMON block: a1=iaea05$au197ng[EN-NRM];.

Monitor point from EXFOR.

Single monitor value is usually given in EXFOR file in COMMON block. This value can be used in an expression referring to Header of the column in the COMMON block by using [Header], e.g. a0=[MONIT1];. So, renormalization by single point can also be described without using intermediate variables, e.g.:

```
y = y * iaea05$au197ng[0.0253] / [MONIT1];
```

Abundance.

When necessary, cross sections can be corrected by using natural abundance of isotopes and cross section of competing reaction. Abundance is coded as abu[isotope], can be used in expressions and will be replaced by value taken from internal library. For example:

```
20388002 m2:rrdf07$ni61nnp; y = y - abu[ni61]/abu[ni60]*m2;
```

Half-life.

If necessary (for long-lived residuals), cross sections can be corrected by using new half-life value, which is coded as t12[isotope]. It can be used in expressions and will be replaced by

value taken from internal library. For example:

```
30449003  y=y*t12[bi207]/38yr;  # converted to y=y*32.9yr/38yr;
```

Examples:

1. `40274002A Y=Y*0.85`

This means: take data from Subentry 40274.002, filter data for reaction with Pointer=<A>; for every data point perform action: multiply data value by factor 0.85

2. Set systematic uncertainties equal to 2% of data for Subentry 10221039

```
10221039 dSys=y*0.02;
```

3. Renormalize data. Define old and new monitors: CS from ENDF-B/IV, reaction U-235(n,f) and modern data from IAEA Standards-2006 library; calculate relative data uncertainty; re-calculate data values using old and monitor; add uncertainty of the new monitor.

```
10221039   m0:endfb4 $ u235nf;    m1:iaeastd2006 $ u235nf;
           dy=dy/y;   y=y/m0*m1;  dy=(dy^2+(dm1/m1)^2)^0.5*y;
```

4. Delete data from energy range from 180 to 265 KeV; multiply data by 0.87; then modify data errors as: previous value plus 5%; set uncertainty of energy equal to 20 KeV

```
41225015  e:1.8e3 265e3; del; e:*;  dy=dy/y;  y=y*0.87;
          dy=dy**2+0.05**2;  dy=dy**0.5*y;  de=2e4;
```

5. Calculate ratios to used monitor: U-235(n,f) from ENDF-B/IV, and produce “right” C4 file

```
10221039 mf=203; m0:endfb4 $ u235nf; Y=Y/m0; dY=dY/m0; A=18.9; dA=92235.9
```

6. Output monitor data on energies of experimental points (for debugging purposes)

```
10221039 m0:endfb4 $ u235nf; y=m0; mt=18;
```

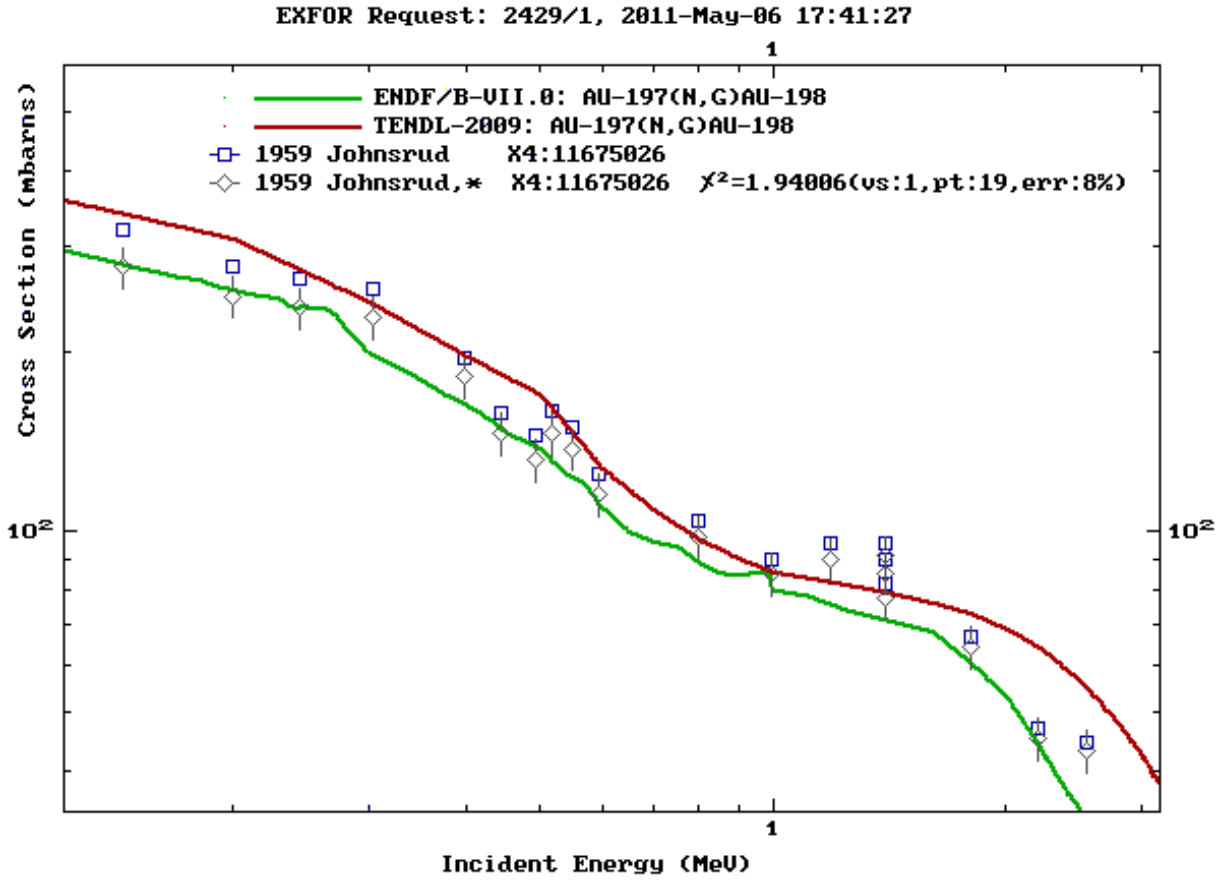
7. Output re-normalization factors (for debugging purposes)

```
10221039 m0:endfb4 $ u235nf;   m1: iaeastd2006 $ u235nf;
         y=m1/m0;  mf=203;  mt=18;
```

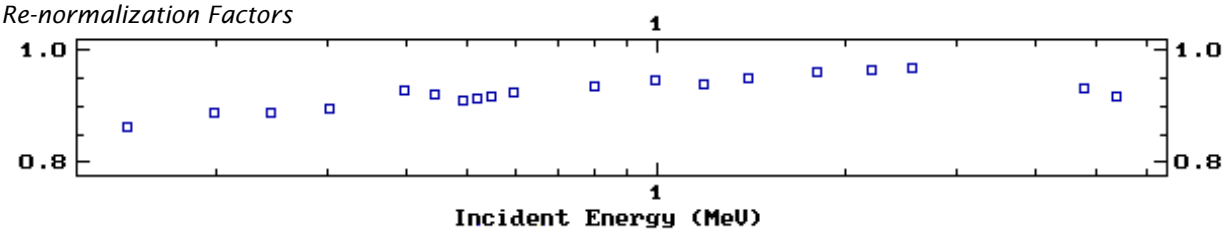
Real examples:

1. Two monitoring points (given in EXFOR COMMON blocks) were used together with energy dependent monitor. Re-normalize absolute cross section data.

```
11675026                                  #dataset=SUBENT
a1=std05$u235nf[EN-NRM]/[MONIT1];         #correction factor for thermal cross section 235U(n,f)
a2=std05$au197ng[EN-NRM]/[MONIT2];        #correction factor for thermal cross section 197Au(n,g)
m0: allen58 $ U235nf;                     #used monitor: 235U(n,f), Allen & Henkel, 1958
m1: std05 $ u235nf;                       #new monitor: 235U(n,f): IAEA-Standard 2005
y =y/a1*a2*m1/m0;                         #re-normalization of data
dy=y*0.08;                                #set up data errors to 8% of data values
```



Re-normalization Factors



2. Re-normalization of data when monitor data are present in original EXFOR.
EXFOR 1142003, Menlove, 1967 Reaction: 25-MN-55(N,G)25-MN-56,,SIG

Describe corrections:

```
SUBENT        11420001     860612
BIB                 11          19
INSTITUTE   (1USALOK)
REFERENCE   (J,PR,163,1299,67)
            (C,66WASH,2,746,6603)
AUTHOR      (H.O.MENLOVE,K.L.COOP,H.A.GRENCH,R.SHER)
TITLE       NEUTRON RADIATIVE CAPTURE CROSS SECTIONS FOR NA23,
            MN55, IN115, AND HO165 IN THE ENERGY REGION 1.0 TO 19.4
            MEV.
FACILITY    (VDG)
INC-SOURCE  (P-T) 1.0-2.2 MEV.
            (D-D) 3.3-6.1 MEV.
            (A-BE) 13.3-19.4 MEV.
            (D-T) 13.3-19.4 MEV.
MONITOR     (92-U-235(N,F),,SIG)
DETECTOR    (NAICR)
METHOD      (ACTIV)
STATUS      (SCSRS)
HISTORY     (760715T) TRANSLATED FROM SCISRS
            (820813A) CONVERTED TO REACTION FORMALISM
            (860612A) BIB UPDATE.
ENDBIB              19
NOCOMMON             0           0
ENDSUBENT           22
SUBENT        11420003     860612
BIB                  2           2
REACTION    (25-MN-55(N,G)25-MN-56,,SIG)
DECAY-DATA  (25-MN-56,2.58HR,DG)
ENDBIB               2
NOCOMMON             0           0
DATA                 5          17
EN          EN-RSL      DATA        DATA-ERR    MONIT
MEV         MEV         B           B           B
 9.70    -01 1.00    -01 2.80    -03 2.2     -04 1.22
 1.56    +00 1.2     -01 1.94    -03 1.5     -04 1.26
 2.15    +00 1.3     -01 1.89    -03 1.4     -04 1.31
 . . . . . . . . . . . . . . . . . . . . . . . . . . .
 1.735   +01 3.2     -01 7.05    -04 7.1     -05 2.30
 1.844   +01 3.3     -01 5.80    -04 5.5     -05 2.18
 1.939   +01 3.5     -01 4.72    -04 4.8     -05 2.11
ENDDATA              19
ENDSUBENT            26
```

Archive of monitors

IAEA Standards-2006

```
#Old and new Monitors:
11420003
   m0: [EN,MONIT];
   m1:iaeastd2006 $ u235nf;
   . . . . . .
   . . . . . .
```

Requested corrections:

```
11420003                          #dataset=SUBENT
   m0: [EN,MONIT];                #old monitor: 235U(n,f) given in EXFOR DATA
   m1: iaeastd2006$u235nf;        #new monitor: 235U(n,f): IAEA-Standard 2006
   dy= dy/y;                      #to relative uncertainties
   y = y/m0*m1;                   #re-normalization of data
   dy= dy^2+dm1^2;                #quadratic summation
   dy= dy^0.5*y;                  #back to absolute uncertainties
```

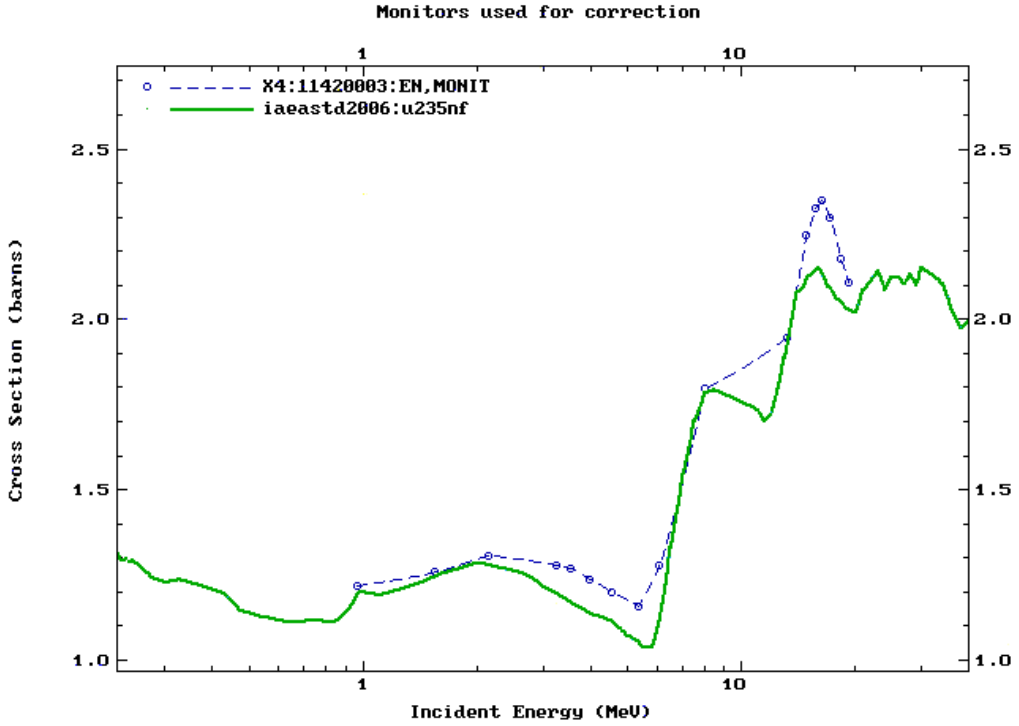
Protocol of executed corrections:

Applied corrections. Datasets: 1

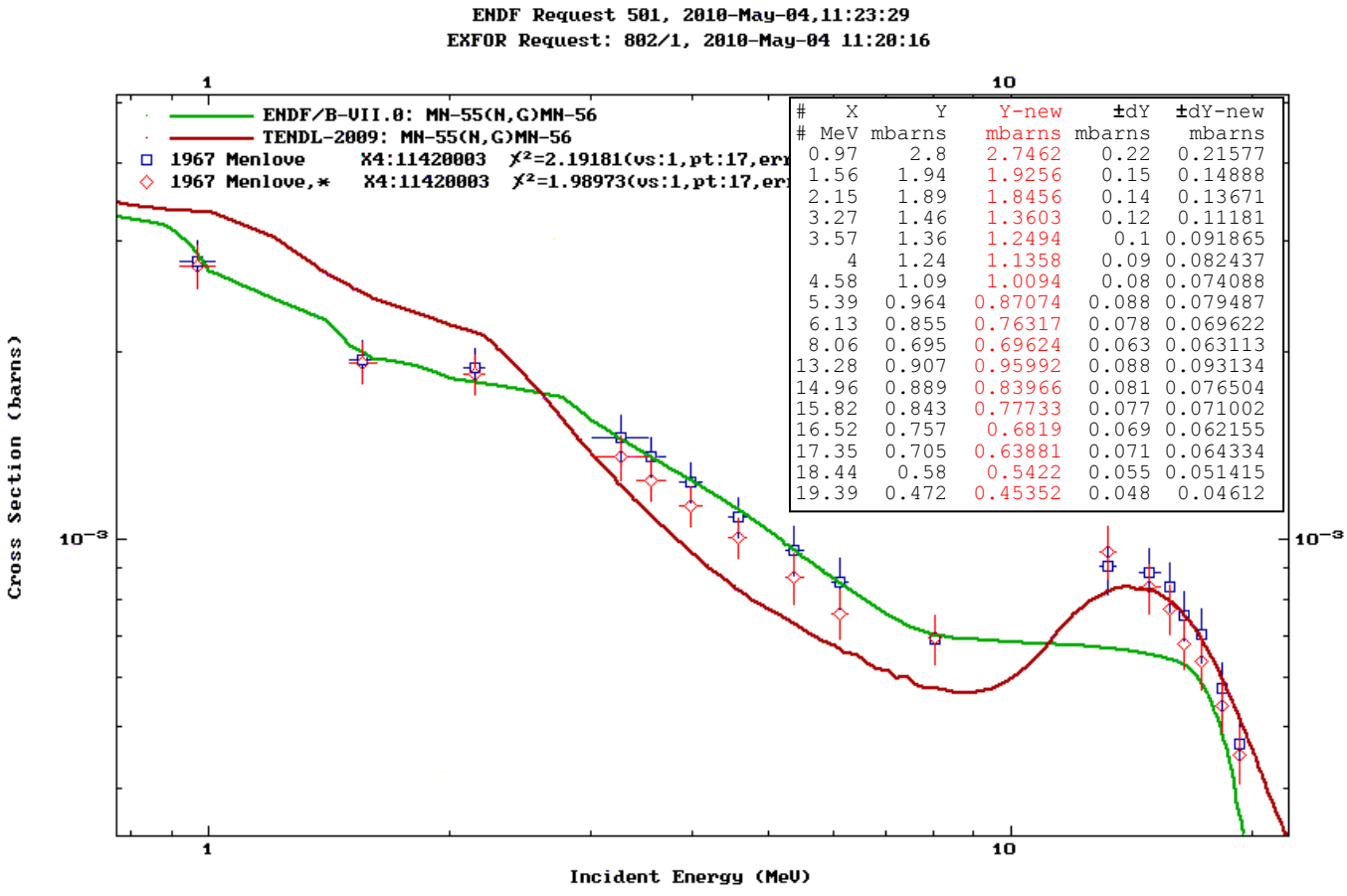
1) EXFOR:#11420003 Ref: H.O.MENLOVE,ET.AL. (67) Corrected_Points:17

11420003 M0:[EN,MONIT]; M1:iaeastd2006$u235nf; dY=dY/Y; Y=Y/M0*M1; dY=dY^2+dM1^2; dY=dY^0.5*Y;

Monitor values:



Final results compared with original data and evaluation data:



# X	Y	Y-new	±dY	±dY-new
# MeV	mbarns	mbarns	mbarns	mbarns
0.97	2.8	2.7462	0.22	0.21577
1.56	1.94	1.9256	0.15	0.14888
2.15	1.89	1.8456	0.14	0.13671
3.27	1.46	1.3603	0.12	0.11181
3.57	1.36	1.2494	0.1	0.091865
4	1.24	1.1358	0.09	0.082437
4.58	1.09	1.0094	0.08	0.074088
5.39	0.964	0.87074	0.088	0.079487
6.13	0.855	0.76317	0.078	0.069622
8.06	0.695	0.69624	0.063	0.063113
13.28	0.907	0.95992	0.088	0.093134
14.96	0.889	0.83966	0.081	0.076504
15.82	0.843	0.77733	0.077	0.071002
16.52	0.757	0.6819	0.069	0.062155
17.35	0.705	0.63881	0.071	0.064334
18.44	0.58	0.5422	0.055	0.051415
19.39	0.472	0.45352	0.048	0.04612

Table 1. Description of corrections.

Element	*Syntax*	*Meaning, comments*
List of corrections	**#**comment **$A** Date, Evaluator Correction . . . . . . Correction	Describes corrections to many datasets. Text starting with **#** will be ignored. **$A** stands for the Author of the correction: when and who made this file.
Correction	DatasetID Instruction**;** …Instruction [Instruction [; Instruction]]	Describes corrections to one dataset; can be presented in several lines
Dataset	`SubentryPointer`	8 or 9 symbols: Entry(5), Subent-No (3 digits), pointer(1). Pointer can be blank.
Instruction	Command	
	Declaration	conditions and parameters
	Calculation	describes how to modify data
Command	`Del;`	Delete data from the Dataset. If energy range is not given – ignore whole dataset.

Declaration	`E: EnMin EnMax;`
	`E: * EnMax;`
	`E: EnMin;`
	`E: *;`
	`E:;` *equivalent to* `E: *;` *and* `E * *;`
		Specify interval of incident energy (eV). EnMin, EnMax are real numbers. Symbol * means no limit. All further manipulations will be done only within this interval.

	`M0: library $ reaction;` *the same for* `M1, M2, M3,…, M7`	Specify files with monitor data which will be used for re-normalizations
	`M0: [EN, MONIT];` *the same for* `M1, M2, M3,…, M7`	Take monitor data from EXFOR file: from columns EN and MONIT
	`M0: [EN, MONIT, MONIT-ERR];`	Take monitor data from EXFOR file: from columns EN, MONIT and uncertainties from MONIT-ERR
	`M0: [EN-MIN ! EN-MAX, MONIT];`	Take monitor data from EXFOR: calculate energy: average value of data from columns EN-MIN and EN-MAX
	`M0: [EN, MONIT:2];`	Take monitor data from EXFOR column MONIT with Pointer='2'
	`X4U: Date;`	Specify date of last update of the given Subentry. To detect, if given corrections are out of date. *Not yet fully supported.*
Calculation	Variable = Expression	
Variable	`E, dE, Y, dY, A, dA, E2, dE2`	Data in C4 file – REAL array [8]
	`MF, MT`	MF, MT in C4 file
	`dSys, dStat`	Systematic and statistical uncertainties.
	`a0, a1, a2, a3, a4, a5, a6, a7,` `c0, c1, c2, c3, c4, c5, c6, Fc`	Intermediate variables
Expression	<Operand>	Parentheses are not allowed; blanks are ignored
	<Operand><operation>...<Operand><operation>...<Operand>	
operation	`^ * / + -` (since 2011 `**` can be used instead of `^`)	Note. a ^ b = a^b
Operand	Variable	See above
	`M0, M1, M2, M3, M4, M5, M6, M7` `dM0,dM1,dM2,dM3,dM4,dM5,dM6,dM7`	Value from monitor interpolated for energy of current data point; the same for monitor-uncertainties (dM0…dM7)

	Number	Numerical value (REAL in Fortran format)
	Number with units	Converted to basic units, e.g. 2min to 2*60, 38yr to 38*31556926. (seconds), 20MeV to 20*1e6 , 2% to 2*0.01
	`[Header]`	Value from EXFOR COMMON block column named "Header", e.g. MONIT2
	`library $ reaction [number]`	Value from monitor for energy=number
	`library $ reaction [Header]`	Value from monitor for energy=value from COMMON block
	`t12[isotope]`	Half-life of given isotope, e.g. t12[Bi207] will be replaced by 32.9yr
	`abu[isotope]`	Natural abundance of given isotope, e.g. abu[Ni60] will be replaced by 26.223%